Linear Algebra and its Applications 436 (2012) 252–261

Contents lists available at SciVerse ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

On the signless Laplacian index of unicyclic graphs with fixed diameter☆

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ARTICLE INFO

Article history:
Received 8 August 2010
Accepted 4 July 2011
Available online 30 July 2011

Submitted by S. Fallat

AMS classification:
05C50
15A18

Keywords:
Unicyclic graph
Signless Laplacian index
Diameter

ABSTRACT

In the paper, we identify graphs with the maximal signless Laplacian spectral radius among all the unicyclic graphs with n vertices of diameter d.

1. Introduction

We consider only simple graphs (i.e. finite, undirected graphs without loops or multiple edges). Let $G = (V_G, E_G)$ be a simple graph on n vertices and m edges (so $n = |V_G|$ is its order, and $m = |E_G|$ is its size). Spectral graph theory [6,11,12] studies properties of graphs using the spectrum of related matrices. The most studied matrix associated with G appears to be adjacency matrix $A = (a_{ij})$ where $a_{ij} = 1$ if v_i and v_j of the graph G are adjacent and 0 otherwise. Another much studied matrix is the Laplacian, defined by $L = D - A$ where D is the diagonal matrix with degrees of the vertices on the main diagonal (see [1,16,24]). The matrix $Q = D + A$ is called the *signless Laplacian matrix* of G (see [7]), which has recently attracted more and more researchers' attention. One reason for this is that the signless Laplacian spectrum seems to be more informative than other commonly used graph matrices [7].

☆ Financially supported by self-determined research funds of CCNU (CCNU09Y01005 and CCNU09Y01018) from the colleges' basic research and operation of MOE and the National Natural Science Foundation of China (Grant No. 11071096).

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0024-3795/$ - see front matter
doi:10.1016/j.laa.2011.07.002

The matrix Q is real symmetric and positive semidefinite, the eigenvalues of Q can be arranged as $q_1(Q) \geqslant q_2(Q) \geqslant \cdots \geqslant q_n(Q) \geqslant 0$, where the largest eigenvalue $q_1(Q)$ is called *Q-index* of graph G. If Q is irreducible (i.e. if G is connected) then $q_1(G)$ is simple, and the corresponding eigenvector can be taken to be positive; any such vector will be called the *Q-Perron vector* of G. In what follows we shall restrict ourselves to connected graphs. For any such graph, let $q_1(G)$ be its Q-index, while $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ its Q-Perron vector (not necessarily a unit one); x_i is also called the weight of the i-th vertex (with respect to $\mathbf{x}$). The *signless Laplacian characteristic polynomial* of G, equal to $\det(xI - Q)$, is denoted by $\psi(G, x)$ (or, for short, by $\psi(G)$).

The study of the largest Q-eigenvalue remains an attractive topic for researchers. In particular, the extremal values of the Q-index for various classes of graphs, and corresponding extremal graphs, have been investigated. A graph G is a *quasi-k-cyclic graph* if it contains a vertex, say r, such that $G - r$ is a k-cyclic graph, i.e. a connected graph with cyclomatic number $k = |E_{G-r}| - |V_{G-r}| + 1$. For example, if $k = 0$; the corresponding graph is a quasi-tree. In [17] quasi-k-cyclic graphs having the largest Q-index are identified for $k \leq 2$. In [29], graphs with maximal Q-index in the class of graphs with given vertex degrees are determined and these results are applied to unicyclic graphs. In [13] graphs with a given number of pendant vertices was considered. Graphs with maximal Q-index and corresponding extremal graphs are determined. For more progress on this line one may refer to [4,5,7–10,13–15,21–23,25–28,30]; and some other spectral theory on Q-matrix, one may refer to survey papers [8–10] and the references therein.

In this paper, we study the signless Laplacian spectral radius of unicyclic graphs with n vertices and diameter d. We determine graphs with the largest signless Laplacian spectral radius among all the unicyclic graphs with n vertices of diameter d. Moreover, if $4 \leqslant d \leqslant n-3$ with $d \equiv 0 \pmod 2$, then we identify unicyclic graphs with n vertices of diameter d having the second largest Q-index.

In order to state our results, we introduce some notation and terminology. Other undefined notation can be found in [3]. Denote by C_n and P_n the cycle and the path with n vertices, respectively. $G - v$, $G - uv$ denote the graph obtained from G by deleting a vertex $v \in V_G$, or an edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex, or edge, is deleted). Similarly, $G + uv$ is a graph that arises from G by adding an edge $uv \notin E_G$, where $u, v \in V_G$. For $uv \in E_G$, let G_{uv} be the graph obtained from G by subdividing the edge uv, that is, by replacing uv with edges uw and wv, where w is an additional vertex. For $v \in V_G$, $d(v)$ denotes the degree of vertex v and $N(v)$ denotes the set of all neighbors of vertex $v \in V_G$.

A *pendant vertex* is a vertex of degree 1 and a pendant edge is an edge incident with a pendant vertex. Let $PV_G = \{v : d_G(v) = 1\}$. For two vertices u and v $(u \neq v)$, the distance between u and v is the number of edges in a shortest path joining u and v. The diameter of a graph is the maximum distance between any two vertices of G. Let $P = v_0v_1 \ldots v_s$ $(s \geqslant 1)$ be a path of G with $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If $d(v_0), d(v_s) \geqslant 3$, then we call P an *internal path* of G; if $d(v_0) \geqslant 3$ and $d(v_s) = 1$, then we call P a *pendant path* of G; if the subgraph induced by V_P in G is P itself, i.e. $G[V_P] = P$, then we call P an induced path. Obviously, the shortest path between any two distinct vertices of G is an induced path. We call G a *unicyclic graph* if $m = n + 1$; where n is the number of vertices and m is the number of edges. We will use $\mathscr{U}_n^d$ to denote the set of all the n-vertex unicyclic graph of diameter d.

2. Lemmas

In this section, we list some lemmas which will be used to prove our main results.

Lemma 2.1 [20]. *Let G be a connected graph and $q_1(G)$ be the spectral radius of $Q(G)$. Let u, v be two vertices of G. Suppose $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u)$ and $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $Q(G)$, where x_i corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$. Let G^* be the graph obtained from G by deleting the edges vv_i and adding the edges uv_i $(1 \leqslant i \leqslant s)$, If $x_u \geqslant x_v$, then $q_1(G) < q_1(G^*)$.*

Lemma 2.2 [8]. *Let G_{uv} be the graph obtained from a connected graph G by subdividing its edge uv. Then the following holds:*

(i) *if* uv *belongs to an internal path then* $q_1(G_{uv}) < q_1(G)$;
(ii) *if* $G \ncong C_n$ *for some* $n \geq 3$, *and if* uv *is not on the internal path then* $q_1(G_{uv}) > q_1(G)$. *Otherwise, if* $G \cong C_n$ *then* $q_1(G_{uv}) = q_1(G) = 4$.

Lemma 2.3 [19]. *Let* G *be a connected graph and let* $e = uv$ *be a non-pendant edge of* G *with* $N(u) \bigcap N(v) = \emptyset$. *Let* G^* *be the graph obtained from* G *by deleting the edge* uv, *identifying* u *with* v, *and adding a new pendant edge to* $u\ (= v)$. *Then* $q_1(G) < q_1(G^*)$.

Lemma 2.4 [23]. *Let* G *be a connected graph with at least one edge,* Δ *be its maximal degree,* d_i *be the degree of vertex* v_i *and* $m_i = \sum_{v_j \in N_G(v_i)} d_j/d_i$, *then*

(i) $q_1(G) \geqslant \Delta(G) + 1$, *the equality holds if and only if* G *is bipartite and* $\Delta(G) = n - 1$.
(ii) $q_1(G) \leqslant \max\{d_i + m_i \mid v_i \in V_G\}$, *the equality holds if and only if* G *is regular or semi-regular bipartite graph.*

Lemma 2.5 [9]. *Let* u, v *be the adjacent vertices of a connected graph* G, *each of the vertices* u *and* v *has degree at least two, and suppose that two new paths* $P : uu_1u_2 \ldots u_k$, *and* $Q : vv_1v_2 \ldots v_m$ *of length* k, m $(k \geqslant m \geqslant 1)$ *are attached to* G *at* u *and* v, *respectively, to form a new graph* $G_{k,m}$, *where* $u_1, u_2, \ldots, u_k$ *and* $v_1, v_2, \ldots, v_m$ *are distinct new vertices. then* $q_1(G_{k,m}) > q_1(G_{k+1,m-1})$.

Let $Q_v(G)$ denote the principal submatrix of $Q(G)$ obtained by deleting the row and column corresponding to the vertex v. Let $G = G_1u : vG_2$ be the graph obtained from two disjoint graphs G_1 and G_2 by joining a vertex u of graph G_1 to a vertex v of the graph G_2 by an edge. We call G a *connected sum* of G_1 at u and G_2 at v.

Lemma 2.6 [18,21]. *Let* G_1 *and* G_2 *be two graphs.*

(i) *Let* $G = G_1u : vG_2$ *be a connected sum of* G_1 *at* u *and* G_2 *at* v, *then*

$$\psi(G) = \psi(G_1)\psi(G_2) - \psi(G_1)\psi(Q_v(G_2)) - \psi(G_2)\psi(Q_u(G_1)).$$

(ii) *Let* G *be a connected graph with* n *vertices which consists of a subgraph* H *(with at least two vertices) and* $n- \mid H \mid$ *distinct pendant edges (not in* H*) attaching to a vertex* v *in* H. *Then*

$$\psi(G) = (x-1)^{n-|H|}\psi(H) - (n- \mid H \mid)x(x-1)^{n-|H|-1}\psi(Q_v(H)).$$

Lemma 2.7.

(i) *If* H *is a proper subgraph of a connected graph* G, *then* $q_1(H) < q_1(G)$.
(ii) *Let* G *be a unicyclic graph of order* n, *then* $q_1(G) \geqslant q_1(C_n)$, *and equality holds if and only if* $G \cong C_n$ $(n \geqslant 3)$.

Proof.

(i) Is a consequence of the well-known theorem on non-negative matrices; see also [2,13].
(ii) If $G \cong C_n$, it is obvious that $q_1(G) = q_1(C_n)$. So we suppose $G \ncong C_n$. By Lemma 2.4, we have

$$q_1(G) \geqslant \Delta(G) + 1 \geqslant 4 = \max\{d(v) + m(v) \mid v \in V(C_n)\} \geqslant q_1(C_n),$$

where the first and second equalities hold if and only if $\Delta(G) = n - 1 = 3$, and G is bipartite. Such graphs do not exist. So we have $q_1(G) > q_1(C_n)$. $\square$

Lemma 2.8 [18]. *Let* G_1 *and* G_2 *be two graphs. If* $\psi(G_2, x) > \psi(G_1, x)$ *for* $x \geqslant q_1(G_2)$, *then* $q_1(G_1) > q_1(G_2)$.

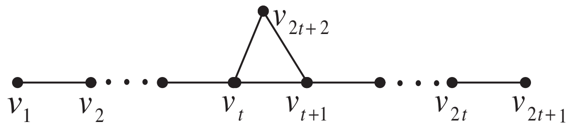

Fig. 1. Graph H_0.

Let $A_v(G)$ (resp. $D_v(G)$) be the principal submatrix of $A(G)$ (resp. $D(G)$) obtained by deleting the row and column corresponding to the vertex v. Then, we have

$$A_v(G) = A(G - v) \text{ and } D_v(G) = D(G - v) + \hat{D}(N_G(v)),$$

where $\hat{D}(N_G(v)) = \mathrm{diag}(d_{11}, d_{22}, \ldots, d_{n-1,n-1})$ is a diagonal matrix with $d_{ii} = 1$ if $v_i \in N_G(v)$ and 0 otherwise, $i = 1, 2, \ldots, n - 1$.

Lemma 2.9. *Let H_0 be the graph as shown in Fig. 1. Suppose that $t \geqslant 2$, then $\psi(Q_{v_{t+1}}(H_0); x) - \psi(Q_{v_t}(H_0); x) = x(x - 2)$.*

Proof. We first calculate the characteristic polynomial of $Q_{v_t}(H_0)$. Since $Q(H_0) = A(H_0) + D(H_0)$, we may conclude that

$$\begin{aligned} Q_{v_t}(H_0) &= A_{v_t}(H_0) + D_{v_t}(H_0) \\ &= A(H_0 - v_t) + D(H_0 - v_t) + \hat{D}(N_G(v_t)) \\ &= q_1(H_0 - v_t) + \hat{D}(\{v_{t-1}, v_{t+1}, v_{t+2}\}). \end{aligned}$$

Because $H_0 - v_t \cong P_{t-1} \bigcup P_{t+2}$, we can get $Q(H_0)$ in which the rows and columns corresponding to the vertices as the ordering $v_t, v_{t-1}, \ldots, v_1, v_{2t+2}, v_{t+1}, v_{t+2}, \ldots, v_{2t+1}$. Furthermore, let $E_{11} = [e_{ij}]$ be a square matrix of order $t - 1$, where $e_{11} = 1$ and $e_{ij} = 0$ whenever $i \neq 1$ and $j \neq 1$; $F_{kk} = [f_{ij}]$ be a square matrix of order $t + 2$, where $f_{kk} = 1$ and $f_{ij} = 0$ whenever $i \neq k$ and $j \neq k$. Then

$$Q_{v_t}(H_0) = \begin{pmatrix} Q(P_{t-1}) + E_{11} & \mathbf{0} \\ \mathbf{0} & Q(P_{t+2}) + F_{11} + F_{22} \end{pmatrix}.$$

Hence,

$$\psi(Q_{v_t}(H_0); x) = \psi(Q(P_{t-1}) + E_{11}; x) \cdot \psi(Q(P_{t+2}) + E_{11} + E_{22}; x).$$

In order to simplify the notation, we denote $\psi(Q(P_{t-1}) + E_{11}; x)$ and $\psi(Q(P_{t+2}) + E_{11} + E_{22}; x)$ by $f_{t-1,1}(x)$ and $f_{t+2,2}(x)$, respectively.

Similarly, we can get that

$$\begin{aligned} \psi(Q_{v_{t+1}}(H_0); x) &= \psi(Q(P_t) + E_{11}; x) \cdot \psi(Q(P_{t+1}) + E_{11} + E_{22}; x) \\ &= f_{t,1}(x) \cdot f_{t+1,2}(x). \end{aligned}$$

In general,

$$f_{n_1,1}(x) = \det \begin{pmatrix} x-2 & -1 & & & \mathbf{0} \\ -1 & x-2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & x-2 & -1 \\ \mathbf{0} & & & -1 & x-1 \end{pmatrix}_{n_1 \times n_1},$$

$$f_{n_2,2}(x)=\det\begin{pmatrix} x-2 & -1 & & & & \mathbf{0} \\ -1 & x-3 & -1 & & & \\ & -1 & x-2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & x-2 & -1 \\ \mathbf{0} & & & & -1 & x-1 \end{pmatrix}_{n_2\times n_2}.$$

Hence, we deduce the recurrence relations

$$f_{n_1,1}(x)=(x-2)f_{n_1-1,1}(x)-f_{n_1-2,1}(x)\quad (n_1\geqslant 2); \tag{2.1}$$

$$\begin{aligned} f_{n_2,2}(x)&=(x-2)[(x-3)f_{n_2-2,1}(x)-f_{n_2-3,1}(x)]-f_{n_2-2,1}(x)\\ &=(x^2-5x+5)f_{n_2-2,1}(x)-(x-2)f_{n_2-3,1}(x)\quad (n_2\geqslant 3). \end{aligned} \tag{2.2}$$

In particular, $f_{0,1}(x)=f_{0,2}(x)=1$. Hence

$$\begin{aligned} \psi(Q_{v_{t+1}}(H_0);x)-\psi(Q_{v_t}(H_0);x) &= f_{t,1}(x)\cdot f_{t+1,2}(x)-f_{t-1,1}(x)\cdot f_{t+2,2}(x)\\ &= f_{t,1}(x)\cdot[(x^2-5x+5)f_{t-1,1}(x)-(x-2)f_{t-2,1}(x)]\\ &\quad -f_{t-1,1}(x)\cdot[(x^2-5x+5)f_{t,1}(x)-(x-2)f_{t-1,1}(x)]\\ &= (x-2)[f_{t-1,1}(x)^2-f_{t,1}(x)\cdot f_{t-2,1}(x)]. \end{aligned}$$

The second equality follows by Eq. (2.2).

Now, we show that $f_{t-1,1}(x)^2-f_{t,1}(x)\cdot f_{t-2,1}(x)=x$, by induction on t.

By direct computing, if $t=2$ we have

$$f_{1,1}(x)^2-f_{2,1}(x)\cdot f_{0,1}(x)=(x-1)^2-(x^2-3x+1)\cdot 1=x.$$

Hence our result holds for $t=2$. Suppose that $f_{t-2,1}(x)^2-f_{t-1,1}(x)\cdot f_{t-3,1}(x)=x$.

$$\begin{aligned} f_{t-1,1}(x)^2-f_{t,1}(x)\cdot f_{t-2,1}(x) &= f_{t-1,1}(x)^2-f_{t-2,1}(x)\cdot[(x-2)f_{t-1,1}(x)-f_{t-2,1}(x)]\\ &= f_{t-1,1}(x)^2-(x-2)f_{t-2,1}(x)f_{t-1,1}(x)+f_{t-2,1}(x)^2\\ &= f_{t-1,1}(x)^2-(x-2)f_{t-2,1}(x)f_{t-1,1}(x)\\ &\quad +[f_{t-1,1}(x)\cdot f_{t-3,1}(x)+x]\quad \text{(by induction)}\\ &= x+f_{t-1,1}(x)^2-f_{t-1,1}(x)[(x-2)f_{t-2,1}(x)-f_{t-3,1}(x)]\quad \text{(by (2.1))}\\ &= x. \end{aligned}$$

So we have $\psi(Q_{v_{t+1}}(H_0);x)-\psi(Q_{v_t}(H_0);x)=x(x-2)$, as desired. □

For $G\in\mathscr{U}_n^d$, we have $n\geqslant 3$ and $1\leqslant d\leqslant n-2$. If $d=1$, then $G\cong C_3$. Therefore, in the following, we assume that $d\geqslant 2$ and $n\geqslant 4$.

Let Δ_n^d be a graph of order n obtained from a triangle by attaching $n-d-2$ pendant edges and a path of length $\lfloor d/2\rfloor$ at one vertex of the triangle, and a path of length $\lceil d/2\rceil-1$ to another vertex of the triangle, respectively.

Let ∇_n^d be a graph of order n obtained from a triangle by attaching $n-d-2$ pendant edges and a path of length $\lceil d/2\rceil-1$ at one vertex of the triangle, and a path of length $\lfloor d/2\rfloor$ to another vertex of the triangle, respectively.

Note that if $d=n-2$ or $d\equiv 1\pmod 2$, then $\Delta_n^d\cong\nabla_n^d$.

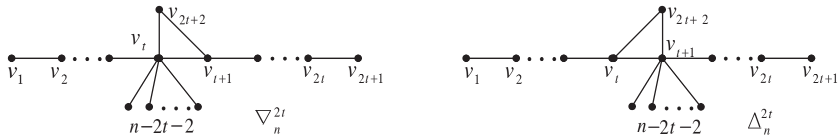

Fig. 2. Graphs ∇_n^{2t} and Δ_n^{2t}.

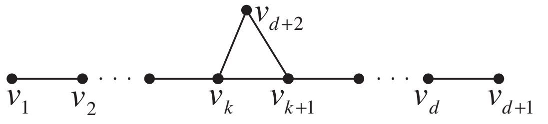

Fig. 3. Graph U_0.

Lemma 2.10. *Let Δ_n^{2t} and ∇_n^{2t} be the above two graphs shown in Fig. 2. Suppose that $2 \leqslant t \leqslant \left\lfloor \frac{n-3}{2} \right\rfloor$. Then $q_1(\Delta_n^{2t}) > q_1(\nabla_n^{2t})$.*

Proof. We first show that $\psi(\nabla_n^{2t}; x) > \psi(\Delta_n^{2t}; x)$ for $x \geqslant q_1(\nabla_n^{2t})$. By direct computation (based on Lemma 2.6(ii)) we get,

$$\psi(\nabla_n^{2t}; x) = (x-1)^{n-2t-2}\psi(H_0) - (n-2t-2)x(x-1)^{n-2t-3}\psi(Q_{v_t}(H_0); x);$$

$$\psi(\Delta_n^{2t}; x) = (x-1)^{n-2t-2}\psi(H_0) - (n-2t-2)x(x-1)^{n-2t-3}\psi(Q_{v_{t+1}}(H_0); x).$$

Note that by Lemma 2.4(i), we have $q_1(\nabla_n^{2t}) > 2$, hence in view of Lemma 2.9, we have

$$\begin{aligned}\psi(\nabla_n^{2t}; x) - \psi(\Delta_n^{2t}; x) &= (n-2t-2)x(x-1)^{n-2t-3}[\psi(Q_{v_{t+1}}(H_0); x) - \psi(Q_{v_t}(H_0); x)] \\ &= (n-2t-2)x^2(x-1)^{n-2t-3}(x-2) \\ &> 0\end{aligned}$$

for $x \geqslant q_1(\nabla_n^{2t})$.

By Lemma 2.8, we get $q_1(\Delta_n^{2t}) > q_1(\nabla_n^{2t})$, as desired. $\square$

Let U_0 be the unicyclic graph of order $d+2$ shown in Fig. 3. Let $U_0(p_2, \ldots, p_d, p_{d+2})$ be a graph of order n obtained from U_0 by attaching p_i pendant vertices to each $v_i \in V(U_0) \setminus \{v_1, v_{d+1}\}$, respectively, where $p_{d+2} = 0$ when $k = 1$ or $k = d$. Denote

$$\widetilde{\mathscr{U}}_n^d = \left\{ U_0(p_2, \ldots, p_d, p_{d+2}) : \sum_{i=2}^{d} p_i + p_{d+2} = n-d-2 \right\}$$

and $\bar{\mathscr{U}}_n^d = \{U_0(0, \ldots, 0, p_i, 0, \ldots, 0) : p_i \geqslant 0\}$.

Lemma 2.11. *Let $G \in \widetilde{\mathscr{U}}_n^d \setminus \bar{\mathscr{U}}_n^d$. Then there is a graph $G^* \in \bar{\mathscr{U}}_n^d$ such that $q_1(G^*) > q_1(G)$.*

Proof. Let $G \in \widetilde{\mathscr{U}}_n^d \setminus \bar{\mathscr{U}}_n^d$ and $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ the Perron vector of $q_1(G)$, where x_i corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$. Let $t = |\{p_i : p_i \neq 0\}|$. Then $t \geqslant 2$. Let $p_i, p_j \neq 0$, $i < j$. Assume, without loss of generality, that $x_i \geqslant x_j$. Let $N(v_j) \bigcap PV_G = \{u_1, u_2, \ldots, u_{p_j}\}$. Let

$$G_1^* = G - v_j u_1 - \cdots - v_j u_{p_j} + v_i u_1 + \cdots + v_i u_{p_j}.$$

By Lemma 2.1, we have $q_1(G_1^*) > q_1(G)$. Note that $G_1^* \in \bar{\mathscr{U}}_n^d$ for $t = 2$ and $G_1^* \in \widetilde{\mathscr{U}}_n^d \setminus \bar{\mathscr{U}}_n^d$ for $t > 2$. If $t > 2$, then we will use G_1^* to repeat the above step until the cardinality of p_i, being nonzero, is only one. So we have $G_2^*,\ G_3^*,\ldots,G_{t-1}^*$ and $q_1(G_1^*) < q_1(G_2^*) < \ldots < q_1(G_{t-1}^*)$. Note that $G_{t-1}^* \in \bar{\mathscr{U}}_n^d$, and hence the lemma holds. □

Lemma 2.12. *For any graph $G \in \widetilde{\mathscr{U}}_n^d$, $3 \leqslant d \leqslant n-2$, we have $q_1(G) \leqslant q_1(\Delta_n^d)$, and equality holds if and only if $G \cong \Delta_n^d$.*

Proof. Let $G \in \widetilde{\mathscr{U}}_n^d$, $3 \leqslant d \leqslant n-1$ and $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ the Perron vector of $q_1(G)$, where x_i corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$.

Choose $G \in \widetilde{\mathscr{U}}_n^d$ such that the Q-index of G is as large as possible. Then by Lemma 2.11, we can assume that $G \in \bar{\mathscr{U}}_n^d$. Let $N(v_i) \bigcap PV_G = \{u_1, u_2, \ldots, u_t\}$ if $p_i > 0$, $P = v_1v_2\ldots v_kv_{k+1}\ldots v_dv_{d+1}$ be an induced path of G and $C = v_kv_{k+1}v_{d+2}v_k$ the only cycle of G (see Fig. 3). Since $\min\{d(v_1), d(v_{d+1})\} = 1$, we assume $d(v_1) = 1$, $k \neq 1$. The following facts play a crucial role.

Fact 1. *If $p_i > 0$, then $i \in \{k, k+1\}$.*

Proof. Assume to the contrary. We first consider the case $v_i \in V_P \setminus V_C$. Since $G \in \bar{\mathscr{U}}_n^d$, and in this case, G cannot be regular and semi-regular bipartite, by Lemma 2.4(ii),

$$\begin{aligned} q_1(G) &< \max\{\max\{d(v)+m(v) \mid v \in V_G\} \mid G \in \bar{\mathscr{U}}_n^d \ \textit{with}\ q_i > 0, i \notin \{k, k+1, d+2\}\} \\ &= n-d+\frac{(n-d-2)+2+3}{n-d} \\ &\leqslant n-d+2 \\ &= \Delta(\Delta_n^d)+1 \\ &< q_1(\Delta_n^d) \end{aligned}$$

for $n-d-2 \geqslant 1$, a contradiction.

Hence we have $i = d+2$. Let

$$G^* = \begin{cases} G - v_iu_1 - \cdots - v_iu_t + v_ku_1 + \cdots + v_ku_t, & x_k \geqslant x_i; \\ G - v_{k-1}v_k + v_{k-1}v_i, & x_k < x_i. \end{cases}$$

Then, in all cases, $G^* \in \bar{\mathscr{U}}_n^d$. Thus by Lemma 2.1, $q_1(G^*) > q_1(G)$, a contradiction. □

Fact 2. $k = \lceil d/2 \rceil$.

Proof. Otherwise, let

$$G^* = \begin{cases} G - v_dv_{d+1} + v_1v_{d+1}, & k < \lceil d/2 \rceil; \\ G - v_1v_2 + v_{d+1}v_1, & k > \lceil d/2 \rceil. \end{cases}$$

Then, in all cases, $G^* \in \bar{\mathscr{U}}_n^d$. Thus by Lemma 2.5, $q_1(G^*) > q_1(G)$, a contradiction. □

By Facts 1 and 2, we have $G \in \{\nabla_n^d, \Delta_n^d\}$. Thus by Lemma 2.10, our result holds . □

From the proof of Lemmas 2.11 and 2.12, we have

Lemma 2.13. *For $G \in \widetilde{\mathscr{U}}_n^d \setminus \{\Delta_n^d\}$ with $d \equiv 0 \pmod 2$ and $4 \leqslant d \leqslant n-3$, we have $q_1(G) \leqslant q_1(\nabla_n^d)$ and equality holds if and only if $G \cong \nabla_n^d$.*

3. Main results

In this section, we give our two central observations.

Theorem 3.1. *Let G be a graph in $\mathscr{U}_n^d$, $d \geqslant 1$. Then $q_1(G) \leqslant q_1(\Delta_n^d)$, and equality holds if and only if $G \cong \Delta_n^d$.*

Proof. Let $G \in \mathscr{U}_n^d$ and $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ the Perron vector of $q_1(G)$, where x_i corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$.

If $d = 1$, then $G \cong C_3$. If $d = 2$, then $G \cong C_4$, $G \cong C_5$ or $G \cong \Delta_n^2$. Thus by Lemma 2.7, our result holds for $d = 1, 2$. Therefore, in the following, we can assume that $3 \leqslant d \leqslant n - 2$.

Choose $G \in \mathscr{U}_n^d$ such that the Q-index of G is as large as possible. Then, by Lemma 2.7, we can assume that $G \ncong C_n$. Let $P_d = v_1v_2 \ldots v_{d+1}$ be the induced path of length d and let C_q be the only cycle in G. Since $G \ncong C_n$, we have $\min\{d(v_1), d(v_{d+1})\} = 1$, say $d(v_1) = 1$. We first show some claims.

Claim 1. $V_{C_q} \bigcap V_{P_d} \neq \emptyset$.

Proof. Otherwise, since G is connected, there exists an only path $P = v_iv_kv_{k+1} \ldots v_{l-1}v_l$ connecting C_q and P_d, where $v_i \in V_{C_q}$,$v_l \in V_{P_d}$ and $v_k, \ldots, v_{l-1} \in V_G \setminus (V_{C_q} \bigcup V_{P_d})$. Let $u_1, \ldots, u_{d(v_l)-1} \in N_G(v_l) \setminus \{v_{l-1}\}$, $w_1, \ldots, w_{d(v_i)-1} \in N_G(v_i) \setminus \{v_k\}$ and

$$G^* = \begin{cases} G - v_lu_1 - \cdots - v_lu_{d(v_l)-1} + v_iu_1 + \cdots + v_iu_{d(v_l)-1}, & x_i \geqslant x_l; \\ G - v_iw_1 - \cdots - v_iw_{d(v_i)-1} + v_lw_1 + \cdots + v_lw_{d(v_i)-1}, & x_i < x_l. \end{cases}$$

Then, in all cases, $G^* \in \mathscr{U}_n^d$. Thus by Lemma 2.1, $q_1(G^*) > q_1(G)$, a contradiction. □

By Claim 1, $V_{C_q} \bigcap V_{P_d} \neq \emptyset$. Denote $C_q = v_kv_{k+1} \ldots v_{l-1}v_lv_{d+2}v_{d+3} \ldots v_sv_k$ $(s \geqslant d + 2)$, where $\{v_k, v_{k+1}, \ldots, v_{l-1}, v_l\} = V_{C_q} \bigcap V_{P_d}$ and $\{v_{d+2}, v_{d+3}, \ldots, v_s\} = V_{C_q} \setminus V_{P_d}$.

Claim 2. $d(v) = 1$ *for* $v \in V_G \setminus (V_{C_q} \bigcup V_{P_d})$.

Proof. Otherwise, let $v_a \in V_G \setminus (V_{C_q} \bigcup V_{P_d})$ with $v_av_i, v_av_b \in E_G$, where $v_i \in V_{C_q} \bigcup V_{P_d}$ and $v_b \in V_G \setminus (V_{C_q} \bigcup V_{P_d})$. Assume $u_1, \ldots, u_{d(v_i)-1} \in N(v_i) \setminus \{v_a\}$. Let

$$G^* = \begin{cases} G - v_av_b - v_iv_b, & x_i \geqslant x_a; \\ G - v_iu_1 - \cdots - v_iu_{d(v_i)-1} + v_au_1 + \cdots + v_au_{d(v_i)-1}, & x_i < x_a. \end{cases}$$

In all cases, $G^* \in \mathscr{U}_n^d$. Thus by Lemma 2.1, $q_1(G^*) > q_1(G)$, a contradiction. □

Claim 3. $k \neq l$.

Proof. Suppose $k = l$. Then $s \geqslant d + 3$ and $k \neq 1, d + 1$. Since $d \geqslant 3$, we can assume that $k \geqslant 3$. Let

$$G^* = \begin{cases} G - v_{d+2}v_{d+3} + v_{k-1}v_{d+3}, & x_{k-1} \geqslant x_{d+2}; \\ G - v_{k-2}v_{k-1} + v_{d+2}v_{k-2}, & x_{k-1} < x_{d+2}. \end{cases}$$

Then in all cases, $G^* \in \mathscr{U}_n^d$. Thus by Lemma 2.1, $q_1(G^*) > q_1(G)$, a contradiction. □

Claim 4. $l = k + 1$, *and* $s - d = 2$.

Proof. We first show that $l = k + 1$. Otherwise, by Claim 3 we have $l - k > 1$. Thus v_{k+1} exists and $v_k v_{k+1} \in E_{C_q} \bigcap E_{P_d}$. Then we will let $\widetilde{G}$ be obtained from G by deleting the edge $v_k v_{k+1}$, identifying v_k with v_{k+1} as a new vertex w_k, and let G^* be obtained from $\widetilde{G}$ by adding a new pendant edge to v_1. So we have $G = \widetilde{G}_{w_k v_{k+2}}$ and $\widetilde{G}$ is a subgraph of G^*. By Lemmas 2.2 and 2.7, $q_1(G) < q_1(\widetilde{G})$, $q_1(\widetilde{G}) < q_1(G^*)$. Hence $q_1(G) < q_1(G^*)$. Note that $G^* \in \mathscr{U}_n^d$. Thus, we get a contradiction.

Now it remains to verify that $s - d = 2$. Otherwise, Since $s - d \geqslant l - k = 1$ and $s \geqslant d + 2$, we suppose $s - d > 2$. Thus v_{s-1} exists. Then we let G^* be obtained from G by deleting the edge $v_k v_s$, identifying v_k with v_s as a new vertex u_k, and adding a new pendant edge to u_k. Note that $G^* \in \mathscr{U}_n^d$. By Lemma 2.3, we have $q_1(G) < q_1(G^*)$, a contradiction. $\square$

By Claims 1–4, $G \in \widetilde{\mathscr{U}}_n^d$. By Lemma 2.12, Theorem 3.1 follows immediately. $\square$

From Lemma 2.13 and the proof of Theorem 3.1, we get the following result.

Theorem 3.2. *Let G be a graph in* $\mathscr{U}_n^d \setminus \{\Delta_n^d\}$. *Suppose that* $d \equiv 0 \pmod 2$ *and* $4 \leqslant d \leqslant n - 3$. *Then* $q_1(G) \leqslant q_1(\nabla_n^d)$, *and equality holds if and only if* $G \cong \nabla_n^d$.

References

[1] W.N. Anderson, T.D. Morely, Eigenvalues of the Laplacian of a graph, Linear and Multilinear Algebra 18 (1985) 141–145.
[2] F. Belardo, E.M.L. Marzi, S.K. Simić, J.F. Wang, On the index of necklaces, Graphs Combin. 26 (2010) 163–172.
[3] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, American Elsevier Publishing Co., New York, 1976.
[4] G.X. Cai, Y.Z. Fan, The signless Laplacian spectral radius of graphs with given chromatic number, Appl. Math. 22 (2009) 161–167.
[5] T.J. Chang, Bit-Shun Tam, Graphs with maximal signless Laplacian spectral radius, Linear Algebra Appl. 432 (7) (2010) 1708–1733.
[6] D.M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Applications, third ed., Johann Ambrosius Barth, Heidelberg, 1995.
[7] D. Cvetković, P. Rowlinson, S. Simić, Signless Laplacians of finite graphs, Linear Algebra Appl. 423 (2007) 155–171.
[8] D. Cvetković, S. Simić, Towards a spectral theory of graphs based on the signless Laplacian, I, Publ. Inst. Math. (Beograd) 85 (99) (2009) 19–33.
[9] D. Cvetković, S. Simić, Towards a spectral theory of graphs based on the signless Laplacian, II, Linear Algebra Appl. 432 (2010) 2257–2272.
[10] D. Cvetković, S. Simić, Towards a spectral theory of graphs based on the signless Laplacian, III, Appl. Anal. Discrete Math. 4 (2010) 156–166.
[11] F.R.K. Chung, Spectral Graph Theory, CBMS Regional Conference Series in Mathematics, vol. 92, Published for the Conference Board of the Mathematical Sciences, Washington, DC, 1997.
[12] E.R. van Dam, W.H. Haemers, Which graphs are determined by their spectrum?, Linear Algebra Appl. 373 (2003) 241–272, (Special Issue on the Combinatorial Matrix Theory Conference, Pohang, 2002).
[13] Y.Z. Fan, D. Yang, The signless Laplacian spectral radius of graphs with given number of pendant vertices, Graphs Combin. 25 (2009) 291–298.
[14] Y.Z. Fan, B.S. Tam, J. Zhou, Maximizing spectral radius of unoriented Laplacian matrix over bicyclic graphs of a given order, Linear and Multilinear Algebra 56 (2008) 381–397.
[15] L. Feng, G. Yu, On three conjectures involving the signless Laplacian spectral radius of graphs, Publ. Inst. Math. (Beograd) 85 (2009) 35–38.
[16] M. Fiedler, A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory, Czechoslovak Math. J. 25 (1975) 607–618.
[17] X. Geng, S. Li, S.K. Simić, On the spectral radius of quasi-k-cyclic graphs, Linear Algebra Appl. 433 (2010) 1561–1572.
[18] A.L. Hou, S.C. Li, Ordering n-vertex unicyclic graphs with matching number q by their largest signless Laplacian eigenvalues, submitted for publication.
[19] S.G. Guo, Ordering trees with n vertices and matching number q by their largest Laplacian eigenvalues, Discrete Math. 308 (2008) 4608–4615.
[20] Y. Hong, X.D. Zhang, Sharp upper and lower bounds for largest eigenvalue of the Laplacian matrix of trees, Discrete Math. 296 (2005) 187–197.
[21] S.C. Li, M.J. Zhang, On the signless Laplacian index of cacti with a given number of pendent vertices, Linear Algebra Appl. (2011), doi:10.1016/j.laa.2011.03.065.
[22] J. Liu, B.L. Liu, The maximum clique and the signless Laplacian eigenvalues, Czechoslovak Math. J. 58 (2008) 1233–1240.
[23] M.H. Liu, B.L. Liu, The signless Laplacian spread, Linear Algebra Appl. 432 (2–3) (2010) 505–514.
[24] R. Merris, Laplacian matrices of graphs: a survey, Linear Algebra Appl. 197/198 (1994) 143–176.
[25] B.S. Tam, Y.Z. Fan, J. Zhou, Unoriented Laplacian maximizing graphs are degree maximal, Linear Algebra Appl. 429 (2008) 735–758.
[26] J.F. Wang, Q.X. Huang, Maximizing the signless Laplacian spectral radius of graphs with given diameter or cut vertices, Linear and Mutilinear Algebra (2011), doi:10.1080/03081087.2010.499363.
[27] G. Yu, On the maximal signless Laplacian spectral radius of graphs with given matching number, Proc. Japan Acad. Ser. A 84 (2008) 163–166.

[28] G.H. Yu, On the maximal signless Laplacian spectral radius of graphs with given matching number, Proc. Japan Acad. Ser. A Math. Sci. 84 (9) (2008) 163–166.
[29] X.D. Zhang, The signless Laplacian spectral radius of graphs with given degree sequences, Discrete Appl. Math. 157 (2009) 2928–2937.
[30] B.X. Zhu, On the signless Laplacian spectral radius of graphs with cut vertices, Linear Algebra Appl. 433 (2010) 928–933.